# Finite volume approximation of a degenerate immiscible two-phase flow model of Cahn-Hilliard type

Clément Cancès, Flore Nabet

# Finite volume approximation of a degenerate immiscible two-phase flow model of Cahn-Hilliard type

Clément Cancès and Flore Nabet

**Abstract** We propose a two-point flux approximation Finite Volume scheme for a model of incompressible and immiscible two-phase flow of Cahn-Hilliard type with degenerate mobility. This model was derived from a variational principle and can be interpreted as the Wasserstein gradient flow of the free energy. The fundamental properties of the continuous model, namely the positivity of the concentrations, the decay of the free energy, and the boundedness of the Boltzmann entropy, are preserved by the numerical scheme. Numerical simulations are provided to illustrate the behavior of the model and of the numerical scheme.

**Key words:** Degenerate Cahn-Hilliard, nonlinear stability

**MSC** (2010)**:** 35K52, 35K65, 65M08, 65M12, 76T99

## 1 Introduction

### *1.1 Description of the model*

We are interested in the simulation of a model representing the flow of two incompressible phases in an open polygonal convex subset $\Omega$ of $\mathbb{R}^d$ and on a

Clément Cancès
Team RAPSODI, Inria Lille – Nord Europe,
40 avenue Halley, 59650 Villeneuve d'Ascq, France
e-mail: clement.cances@inria.fr

Flore Nabet
CMAP, Ecole polytechnique, CNRS, Université Paris-Saclay,
91128, Palaiseau, France,
e-mail: flore.nabet@polytechnique.edu

finite time interval $(0,T)$. Since the fluid is incompressible, its composition is fully described by the *saturations* $(c_i)_{i\in\{1,2\}} \in [0,1]^2$ of the phases (i.e., $c_i$ is the volume ratio of the phase $i$ in the fluid). The algebraic constraint

$$c_1 + c_2 = 1 \quad \text{in } \Omega \times (0,T) =: Q \tag{1}$$

follows. The motion of the phase $i$ is governed by a convection-diffusion

$$\partial_t c_i + \boldsymbol{\nabla} \cdot (c_i \mathbf{v}_i) = 0 \quad \text{in } Q. \tag{2}$$

The *velocity* $\mathbf{v}_i$ of the phase $i$ is supposed to be proportional to the gradient of the *potential* $u_i$ of the phase $i$:

$$\mathbf{v}_i = -\frac{1}{\mu_i} \boldsymbol{\nabla} u_i, \quad \text{in } Q, \tag{3}$$

where $\mu_i > 0$ stands for the viscosity of the phase $i$. The last equation to be prescribed in the bulk $Q$ is obtained by imposing a relationship between the difference of the potentials and the saturations

$$u_1 - u_2 = -\kappa \Delta c_1 + \chi(1 - 2c_1) + \Psi_1 - \Psi_2, \tag{4}$$

where $\kappa$ and $\chi$ are strictly positive parameters (with usually $\kappa << \chi$), where $\Psi_i : \overline{\Omega} \to \mathbb{R}$ are smooth exterior potentials acting on the volume of the phase $i$. For instance, when consider the gravitational potential $\Psi_i(\mathbf{x}) = \rho_i \mathbf{x} \cdot \mathbf{g}$ where $\rho_i$ is the density of the phase $i$ and $\mathbf{g}$ is the gravity acceleration, the term $\Psi_1 - \Psi_2$ represents the buoyancy force of the phase $c_1$. The potentials $u_i$ are defined up to a constant. In order to fix this degree of freedom, we impose that

$$\int_\Omega \overline{u}(\mathbf{x},t) \mathrm{d}\mathbf{x} = 0 \quad \text{for a.e. } t \in (0,T), \quad \text{where } \overline{u} = c_1 u_1 + c_2 u_2. \tag{5}$$

We prescribe initial saturations $c_i^0 \in H^1(\Omega)$ satisfying the constraint

$$c_1^0 + c_2^0 = 1 \quad \text{in } \Omega. \tag{6}$$

We also impose no-flux boundary conditions for each phase

$$-\frac{c_i}{\mu_i} \boldsymbol{\nabla} u_i \cdot \mathbf{n} = 0 \quad \text{on } \partial\Omega \times (0,T) \tag{7}$$

and homogeneous Neumann boundary conditions for the saturations $c_i$, i.e.,

$$\boldsymbol{\nabla} c_i \cdot \mathbf{n} = 0 \quad \text{on } \partial\Omega \times (0,T). \tag{8}$$

*Remark 1 (Link with classical degenerate Cahn-Hilliard model).* Define the total velocity $\mathbf{v}_T$ by $\mathbf{v}_T = c_1 \mathbf{v}_1 + c_2 \mathbf{v}_2$, then it follows from (1)–(2) that

$\boldsymbol{\nabla}\cdot\mathbf{v}_T = 0$. Moreover, (8) ensures that $\mathbf{v}_T\cdot\mathbf{n} = 0$ on the boundary. Then one can check that the equation (2) for $i = 1$ rewrites

$$\partial_t c_1 + \boldsymbol{\nabla}\cdot\left(\frac{c_1}{c_1 + \frac{\mu_1}{\mu_2}(1-c_1)}\mathbf{v}_T - \frac{c_1(1-c_1)}{\mu_2 c_1 + \mu_1(1-c_1)}\boldsymbol{\nabla}\left(u_1 - u_2\right)\right) = 0 \quad (9)$$

where the formula (4) can then be used. This yields a classical degenerate Cahn-Hilliard model [6] as soon as $\mathbf{v}_T \equiv \mathbf{0}$. This property is always fulfilled in the one-dimensional case, but it is no longer the case when $d \geq 2$.

## *1.2 Energy, energy dissipation, and entropy*

The fourth order problem model (1)–(8) described above is closely related to the one studied in [3]. It shares many common features with the classical models of immiscible incompressible two-phase flows in porous media (see for instance [8]). Indeed, both models can be interpreted as Wasserstein gradient flows with singular energies (see [4, 5] for the case of porous media flows and the monograph [2] for a extensive presentation on gradient flows in metric spaces). The justification of this variational structure is not the purpose of this contribution. However, the numerical scheme we present was designed to preserve some important properties of the continuous equations that we highlight now.

The free energy $\mathfrak{E}(\mathbf{c})$ of a configuration $\mathbf{c} = (c_1, c_2) \in H^1(\Omega;[0,1])^2$ is given by

$$\mathfrak{E}(\mathbf{c}) = \int_\Omega \left(\frac{\kappa}{2}|\boldsymbol{\nabla}c_1|^2 \mathrm{d}\mathbf{x} + \chi c_1 c_2 + c_1\Psi_1 + c_2\Psi_2 + E_{\mathrm{cons}}(\mathbf{c})\right)\mathrm{d}\mathbf{x},$$

where the constraint (1) has been introduced in the energy via the term

$$E_{\mathrm{cons}}(\mathbf{c}) = \begin{cases} 0 & \text{if } c_1 + c_2 = 1, \\ +\infty & \text{otherwise.} \end{cases}$$

Multiplying (formally) the equation (2) by $u_i$, integrate over $\Omega$, summing over $i \in \{1,2\}$, and using equations (1) and (4), one gets the following energy dissipation property:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathfrak{E}(\mathbf{c}) = -\sum_{i\in\{1,2\}}\int_\Omega \frac{c_i}{\mu_i}\left|\boldsymbol{\nabla}u_i\right|^2 \mathrm{d}\mathbf{x} \leq 0. \quad (10)$$

In particular, the boundedness of the energy ensures that the solutions to (1)–(8) remain uniformly bounded in $H^1(\Omega)$.

The second crucial estimate in the study of the problem is obtained by multiplying equation (2) by $\mu_i \log(c_i)$, integrating over $Q$, summing over $i \in \{1,2\}$, and using (1) together with (4) to get that

$$\mathfrak{H}(\mathbf{c}(\cdot,T))+\iint_Q \Big(\kappa|\Delta c_1|^2-2\chi|\boldsymbol{\nabla} c_1|^2+\boldsymbol{\nabla} c_1\cdot\boldsymbol{\nabla}(\Psi_1-\Psi_2)\Big)\mathrm{d}\mathbf{x}\mathrm{d}t \le \mathfrak{H}(\mathbf{c}^0)<\infty, \tag{11}$$

where

$$\mathfrak{H}(\mathbf{c}) = \sum_{i\in\{1,2\}} \mu_i \int_\Omega (c_i\log(c_i)-c_i+1)\,\mathrm{d}\mathbf{x} \ge 0.$$

This estimates yields a uniform $L^2(Q)$ bound on $u_1-u_2$, from which we deduce a $L^2((0,T);W^{1,1}(\Omega))$ bound on $\overline{u}$, hence a $L^2((0,T);L^{d/(d-1)}(\Omega))$ bound on $u_i$.

## 2 An implicit two-point flux approximation scheme

We propose to discretize the system (1)–(8) thanks to an implicit Finite Volume scheme with two-point flux approximation. This requires a so-called *admissible mesh* in the sense of [7] with an orthogonality condition as detailed in §2.1. Once this discretization at hand, we define the numerical scheme in §2.2. We show in §2.3 some *a priori* estimates that allow to show the existence of a discrete solution to the scheme.

### *2.1 Admissible discretization of $\Omega\times(0,T)$*

Let us first discretize $\Omega$ into a triplet $\big(\mathcal{T},\mathcal{E},(\mathbf{x}_K)_{K\in\mathcal{T}}\big)$. The set $\mathcal{T}$ of the control volumes is supposed to be made of convex disjoint open subsets $K$ of $\Omega$ such that $\overline{\Omega}=\bigcup_{K\in\mathcal{T}}\overline{K}$. The $d$-dimensional Lebesgue measure of $K$ is denoted by $m_K$. The set $\mathcal{E}$ of the faces is made of elements $\sigma$ that are included in hyperplanes and that have strictly positive $(d-1)$ dimensional Lebesgue measure denoted by $m_\sigma$. For all $K\in\mathcal{T}$, we assume that there exists a subset $\mathcal{E}_K$ of $\mathcal{E}$ such that $\partial K=\bigcup_{\sigma\in\mathcal{E}_K}\overline{\sigma}$, and that there exists at most one element in $\mathcal{E}_K$ included in each hyperplane of $\mathbb{R}^d$. As a consequence, the interface between two control volumes $K$ and $L$ is reduced to at most one edge $\sigma$ denoted by $K|L$. We denote by $\mathcal{E}_{\rm ext}=\{\sigma\in\mathcal{E}\mid\sigma\subset\partial\Omega\}$, $\mathcal{E}_{\rm int}=\mathcal{E}\setminus\mathcal{E}_{\rm ext}$, and $\mathcal{E}_{K,\rm int}=\mathcal{E}_K\cap\mathcal{E}_{\rm int}$. The cell centers $(\mathbf{x}_K)_{K\in\mathcal{T}}$ are such that $\mathbf{x}_K\in K$ for all $K$. Given two neighboring cell $K,L\in\mathcal{T}$, we assume that the straight line $(\mathbf{x}_K,\mathbf{x}_L)$ is orthogonal to the face $\sigma=K|L$. For all $\sigma=K|L\in\mathcal{E}_{\rm int}$, we denote by

$$d_\sigma = \mathrm{dist}(\mathbf{x}_K, \mathbf{x}_L), \quad d_{K,\sigma} = \mathrm{dist}(\mathbf{x}_K, \sigma), \quad d_{L,\sigma} = \mathrm{dist}(\mathbf{x}_L, \sigma), \quad \tau_\sigma = \frac{m_\sigma}{d_\sigma}.$$

Our presentation is restricted to uniform discretizations of the time interval $(0,T)$ only for the ease of presentation. Let $N \geq 1$ denote the number of subintervals of $(0,T)$, and let $\Delta t = T/N$ be the corresponding time step. For $n \in \{0,\ldots,N\}$, we denote by $t_n = n\Delta t$.

In the numerical analysis sketched in §2.3, we are interested in getting uniform bounds on the discrete solutions for families of meshes. To do so, we need to assume regularity on the meshes. More precisely, for all $K \in \mathcal{T}$, we denote by $h_K = \mathrm{diam}(K)$, and by $h = \max_{K\in\mathcal{T}} h_K$. Then we assume that there exist strictly positive constants $\alpha$, $\beta$, and $\gamma$ such that

$$m_K \geq \alpha h_K^d, \quad m_\sigma \geq \beta h_K^{d-1}, \quad d_{K,\sigma} \geq \gamma h_K, \qquad \forall K \in \mathcal{T},\ \forall \sigma \in \mathcal{E}_{K,\mathrm{int}}. \tag{12}$$

## *2.2 Discretization of the equations and the initial data*

The equations (2)–(3) for $i \in \{1,2\}$ are discretized into

$$m_K \frac{c_{i,K}^n - c_{i,K}^{n-1}}{\Delta t} + \sum_{\substack{\sigma\in\mathcal{E}_{K,\mathrm{int}} \\ \sigma = K|L}} \tau_\sigma \left( \frac{c_{i,\sigma}^n}{\mu_i} \left( u_{i,K}^n - u_{i,L}^n \right) \right) = 0,\ \forall K \in \mathcal{T}, \forall n \geq 1. \tag{13}$$

The values $c_{i,\sigma}^n$ ($i \in \{1,2\}$) are defined thanks to a phase-by-phase upwinding [8]:

$$c_{i,\sigma}^n = \begin{cases} c_{i,K}^n & \text{if } u_{i,K}^n - u_{i,L}^n \geq 0, \\ c_{i,L}^n & \text{otherwise.} \end{cases} \tag{14}$$

The equation (1) is discretized into

$$c_{1,K}^n + c_{2,K}^n = 1, \qquad \forall K \in \mathcal{T},\ \forall n \geq 1, \tag{15}$$

while (4) is discretized into: $\forall K \in \mathcal{T}$, $\forall n \geq 1$,

$$u_{1,K}^n - u_{2,K}^n = \frac{\kappa}{m_K} \sum_{\substack{\sigma\in\mathcal{E}_{K,\mathrm{int}} \\ \sigma = K|L}} \tau_\sigma \left( c_{1,K}^n - c_{1,L}^n \right) + \chi(1 - 2c_{1,K}^{n-1}) + \Psi_{1,K} - \Psi_{2,K}. \tag{16}$$

Finally, we prescribe the following discrete counterpart to (5):

$$\sum_{K\in\mathcal{T}} m_K \left( c_{1,K}^n u_{1,K}^n + c_{2,K}^n u_{2,K}^n \right) = 0, \qquad \forall n \geq 1. \tag{17}$$

Finally, the initial data $\mathbf{c}^0$ is discretized into $\left(c_{i,K}^0\right)_{K\in\mathcal{T}}$ by setting

$$c_{i,K}^0 = \frac{1}{m_K}\int_K c_i^0(\mathbf{x})\mathrm{d}\mathbf{x}, \qquad \forall K \in \mathcal{T},\ \forall i \in \{1,2\}. \tag{18}$$

The scheme (13)–(17) yields a nonlinear system. Given $\left(c_{1,K}^{n-1}, c_{2,K}^{n-1}\right)_{K\in\mathcal{T}}$, the existence of a discrete solution $\left(c_{1,K}^n, c_{2,K}^n, u_{1,K}^n, u_{2,K}^n\right)_{K\in\mathcal{T}}$ is far from being obvious. This motivates the analysis carried out in the next section.

## *2.3 Stability and existence of a discrete solution*

We define the piecewise constant approximate solution $\left(c_{1,\mathcal{T}}^{\Delta t}, c_{2,\mathcal{T}}^{\Delta t}, u_{1,\mathcal{T}}^{\Delta t}, u_{2,\mathcal{T}}^{\Delta t}\right)$ by setting $c_{i,\mathcal{T}}^{\Delta t}(\mathbf{x},t) = c_{i,K}^n$ and $u_{i,\mathcal{T}}^{\Delta t}(\mathbf{x},t) = u_{i,K}^n$ if $(\mathbf{x},t) \in K \times (t_n, t_{n+1}]$. We also set $c_{i,\mathcal{T}}^{\Delta t}(\mathbf{x},0) = c_{i,K}^0$ for all $\mathbf{x} \in K$.

We first state a $L^\infty(Q)$ *a priori* estimate on the phase saturations:

$$0 \le c_{i,\mathcal{T}}^{\Delta t} \le 1, \qquad \forall i \in \{1,2\}. \tag{19}$$

It can be proved thanks to a simple contradiction argument (see, e.g., [1]).

Define the discrete energy $\mathfrak{E}_{\mathcal{T}}^n \simeq \mathfrak{E}(\mathbf{c}(\cdot,t_n))$ by

$$\mathfrak{E}_{\mathcal{T}}^n = \frac{\kappa}{2}\sum_{\sigma=K|L}\tau_\sigma\left(c_{1,K}^n - c_{1,L}^n\right)^2 + \chi\sum_{K\in\mathcal{T}} m_K c_{1,K}^n c_{2,K}^n + \sum_{i\in\{1,2\}}\sum_{K\in\mathcal{T}} m_K c_{i,K}^n \Psi_{i,K},$$

then the following estimate is a discrete counterpart to (10):

$$\mathfrak{E}_{\mathcal{T}}^n \le \mathfrak{E}_{\mathcal{T}}^n + \Delta t \sum_{i\in\{1,2\}}\frac{1}{\mu_i}\sum_{\sigma=K|L}\tau_\sigma c_{i,\sigma}^n\left(u_{i,K}^n - u_{i,L}^n\right)^2 \le \mathfrak{E}_{\mathcal{T}}^{n-1}, \quad \forall n \ge 1. \tag{20}$$

Its proof consists in multiplying (13) by $\Delta t u_{i,K}^n$, on summing over $K \in \mathcal{T}$, and on using the relations (15) and (16) together with a convexity inequality.

The next estimate is a discrete counterpart to $\iint_Q |\Delta c_1|^2 \mathrm{d}\mathbf{x}\mathrm{d}t \le C$ that can be deduced from (11):

$$\sum_{n=1}^N \Delta t \sum_{K\in\mathcal{T}} m_K \left(\frac{1}{m_K}\sum_{\sigma\in\mathcal{E}_K}\tau_\sigma\left(c_{1,K}^n - c_{1,L}^n\right)\right)^2 \le C. \tag{21}$$

To derive (21), we multiply (13) by $\mu_i \log(c_{i,K}^n)\Delta t$, sum over $K \in \mathcal{T}$ and $n \in \{1,\dots,N\}$, and then combine it with elementary convexity inequalities and a discrete $L^\infty((0,T);H^1(\Omega))$ estimate on $c_{1,\mathcal{T}}^{\Delta t}$ that follows from (20). As a first consequence of (21), one gets a uniform $L^2(Q)$ bound on $u_{1,\mathcal{T}}^{\Delta t} - u_{2,\mathcal{T}}^{\Delta t}$. Moreover, because of (21) and of the regularity of the mesh prescribed in (12), we can prove that, provided the ratio $\Delta t/h^{4-d}$ is large enough, one has

$$c_{1,\sigma}^n + c_{2,\sigma}^n \geq c_\star > 0, \quad \forall n \geq 1, \forall \sigma \in \mathcal{E}_{\rm int}. \tag{22}$$

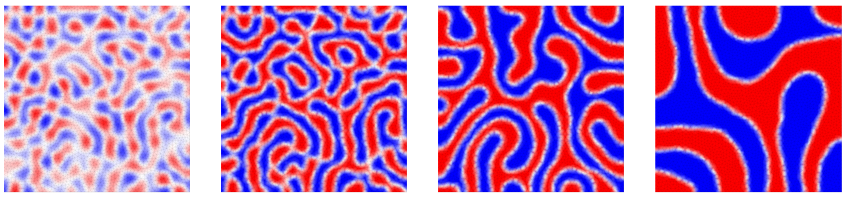
Together with (17), this allows to derive uniform $L^2((0,T); L^{\frac{d}{d-1}}(\Omega))$ bounds on the phase potentials $u_{i,\mathcal{T}}^{\Delta t}$. The following proposition states the existence of (at least) one solution to the scheme (13)–(17).

**Proposition 1 (existence of a discrete solution).** *Assume that the ratio $\Delta t/h^{d-4}$ is large enough, then there exists (at least) one solution $\left(c_{1,K}^n, c_{2,K}^n, u_{1,K}^n, u_{2,K}^n\right)_{K\in\mathcal{T}}$ to the scheme* (13)–(17). *Moreover, it satisfies the* a priori *estimates* (19)–(21).

## 3 Numerical illustration

We present now a numerical simulation on a phase separation dynamics. The initial saturation $c_1^0$ is a random initial concentration with a fluctuation between 0.49 and 0.51, whereas $c_2^0$ is determined by (6). The computational domain $\Omega$ is the square $(0,1)^2$. We consider a triangular mesh whose mesh size $h$ is approximately equal to 0.03. For any control volume $K$, the cell center $\mathbf{x}_K$ is the circumcenter of the triangle $K$. The final time is $t_{\rm f} = 1$ and we choose a fixed time step $\Delta t = 5 \cdot 10^{-5}$. The viscosities which appear in (3) are constant equal to 1 ($\mu_1 = \mu_2 = 1$) and we choose the parameters appearing in (4) as follows: $\kappa = 3 \cdot 10^{-4}$ and $\chi = 0.96$. The exterior potentials $\Psi_1$ and $\Psi_2$ are both put to 0.

First, we represent the saturation $c_1$ in $\Omega$ for different times (see Fig. 1). The pure phase $c_1 = 0$ appears in blue, the homogeneous saturation $c_1 = 0.5$ in white and the pure phase $c_1 = 1$ in red.



(a) $t = 0.006$ (b) $t = 0.01$ (c) $t = 0.05$ (d) $t = 1$

Fig. 1: Approximate saturation $c_{1,\mathcal{T}}^{\Delta t}(\cdot, t)$ in $\Omega$ for different times $t$.

We recover the expected behaviour of the phase separation process. Indeed, at first, the material becomes quickly inhomogeneous, the two components spontaneously separate and form several distinct regions consisting of pure phases (see Fig. 1a). Then, on a slower time scale, the pure phases gather

together to form larger patterns (see Fig. 1b–1d). Moreover, throughout the simulation the saturations $c_1$ and $c_2$ remain bounded between 0 and 1.

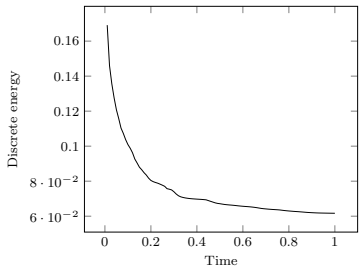



Fig. 2: Evolution of the discrete energy along time.

In Fig. 2, we illustrate that the numerical method dissipates the discrete energy, as predicted by (20). In our simulations, the condition (22) was fulfilled with $c_\star \simeq 0.171$.

**Acknowledgements** This work was carried out in the framework of the project GEOPOR (ANR-13-JS01-0007-01) supported by the French National Agency for Research. The authors also acknowledge the support of the LabEx CEMPI (ANR-11-LABX-0007-01).

## References

1. Ait Hammou Oulhaj, A., Cancès, C., Chainais-Hillairet, C.: Numerical analysis of a nonlinearly stable and positive Control Volume Finite Element scheme for Richards equation with anisotropy (2016). HAL: hal-01372954
2. Ambrosio, L., Gigli, N., Savaré, G.: Gradient flows in metric spaces and in the space of probability measures, second edn. Lectures in Mathematics ETH Zürich. Birkhäuser Verlag, Basel (2008)
3. Barrett, J.W., Blowey, J.F., Garcke, H.: On fully practical finite element approximations of degenerate Cahn-Hilliard systems. M2AN Math. Model. Numer. Anal. **35**(4), 713–748 (2001)
4. Cancès, C., Gallouët, T.O., Monsaingeon, L.: The gradient flow structure of immiscible incompressible two-phase flows in porous media. C. R. Acad. Sci. Paris Sér. I Math. **353**, 985–989 (2015)
5. Cancès, C., Gallouët, T.O., Monsaingeon, L.: Incompressible immiscible multiphase flows in porous media: a variational approach (2016). HAL: hal-01345438
6. Elliott, C.M., Garcke, H.: On the Cahn-Hilliard equation with degenerate mobility. SIAM J. Math. Anal. **27**(2), 404–423 (1996)
7. Eymard, R., Gallouët, T., Herbin, R.: Finite volume methods. Ciarlet, P. G. (ed.) et al., in Handbook of numerical analysis. North-Holland, Amsterdam, pp. 713–1020 (2000)
8. Eymard, R., Herbin, R., Michel, A.: Mathematical study of a petroleum-engineering scheme. M2AN Math. Model. Numer. Anal. **37**(6), 937–972 (2003)